

1,5-Dimethyl-6-phenyl-1,6-dihydro-3-pyridinecarbonitrile  
27531-49-3 | DTXSID30297547

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $7.10 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $1.53 \times 10^{-1}$

**Confidence level:**  $7.65 \times 10^{-1}$

## Nearest Neighbors from the Training Set

Image not found

2-Methyl-p-benzoquinone

**Measured:**  $2.35 \times 10^{-11}$

**Predicted:**  $2.15 \times 10^{-11}$

Image not found

1,3,5-Cycloheptatriene

**Measured:**  $9.69 \times 10^{-11}$

**Predicted:**  $1.00 \times 10^{-10}$